

=> file casreact

FILE 'CASREACT' ENTERED AT 16:41:10 ON 10 MAY 2007

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FILE CONTENT:1840 - 5 May 2007 VOL 146 ISS 20

New CAS Information Use Policies, enter HELP USAGETERMS for details.

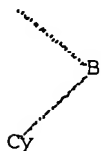
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*****
*
*   CASREACT now has more than 12 million reactions
*
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d stat que L8

L3 STR



Structure attributes must be viewed using STN Express query preparation:
Uploading L3.str

L4 39926 SEA FILE=REGISTRY SSS FUL L3
L5 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L5.str

L6 3643 SEA FILE=CASREACT ABB=ON PLU=ON L4
L8 13 SEA FILE=CASREACT SUB=L6 SSS FUL L5 (79 REACTIONS)

100.0% DONE 492 VERIFIED 79 HIT RXNS 13 DOCS
SEARCH TIME: 00.00.01

ACCESSION NUMBER: 112:139083 CASREACT Full-text

TITLE: Studies on antitumor boron compounds. V. Fluorine- and methoxy-substituted diphenylboron chelates with N,O-bidentate ligands

AUTHOR(S): Yuan, Guozheng; Pang, Jinxin; Zhang, Guomin; Zeng, Fanbo

CORPORATE SOURCE: Dep. Chem., Wuhan Univ., Wuhan, Peop. Rep. China

SOURCE: Youji Huaxue (1989), 9(3), 226-9

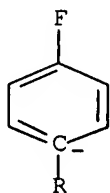
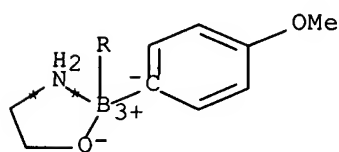
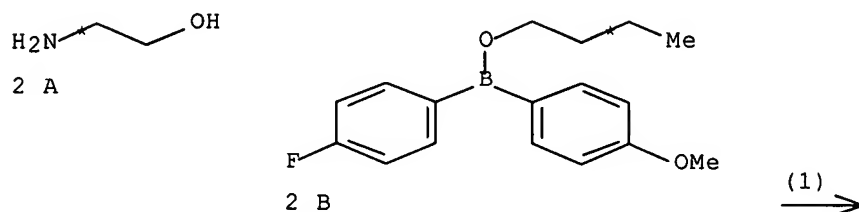
CODEN: YCHHDX; ISSN: 0253-2786

DOCUMENT TYPE: Journal

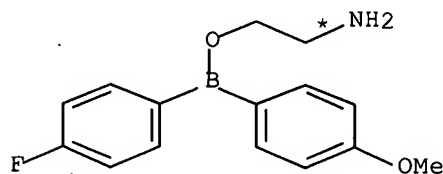
LANGUAGE: Chinese

AB Title diphenylboron chelates of ethanolamine, 2-amino-1-butanol, dl-norvaline, dl-norleucine, dl-phenylalanine, and 8-hydroxyquinoline were prepared Their antitumor effects on mice were tested.

RX(1) OF 41 ...2 A + 2 B ==> C + D

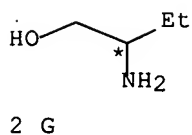
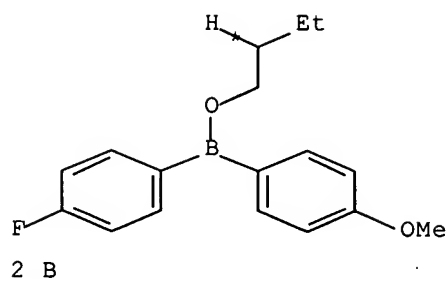


C
YIELD 92%

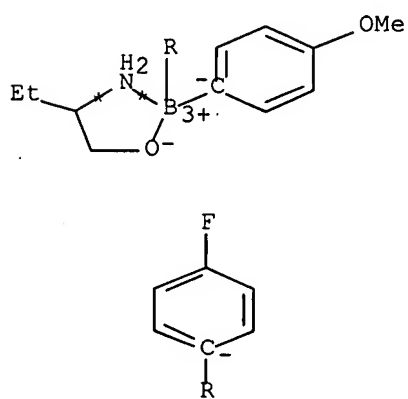


D
YIELD 92%

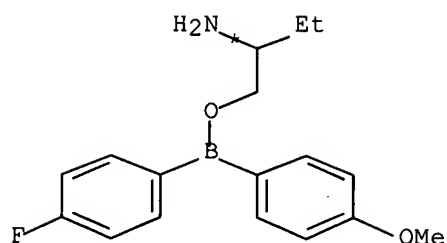
RX(2) OF 41 ...2 B + 2 G ==> H + I



(2) →

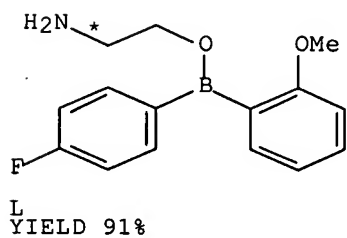
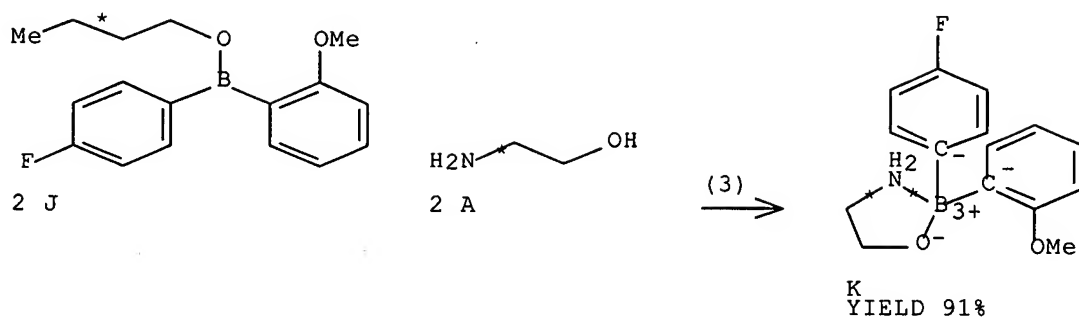


H
YIELD 73%



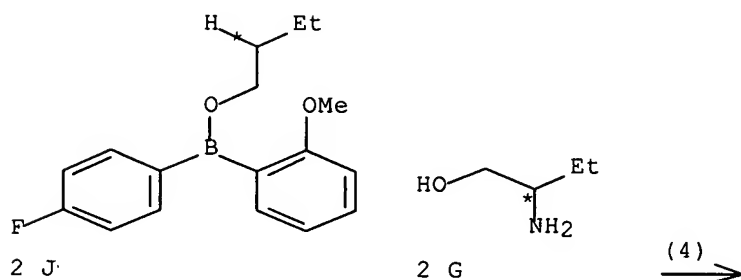
I
YIELD 73%

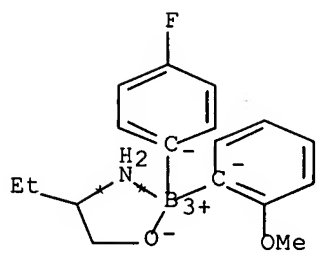
RX(3) OF 41 ...2 J + 2 A ==> K + L



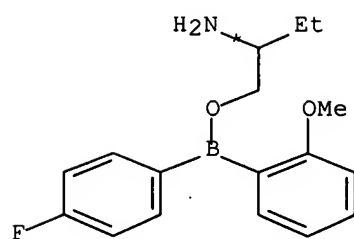
RX(3) RCT J 100689-51-8, A 141-43-5
 PRO K 125842-39-9, L 125553-29-9
 SOL 64-17-5 EtOH, 7732-18-5 Water

RX(4) OF 41 ...2 J + 2 G ==> M + N



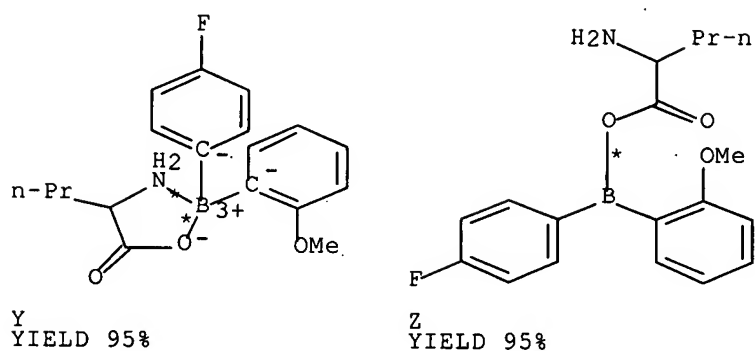
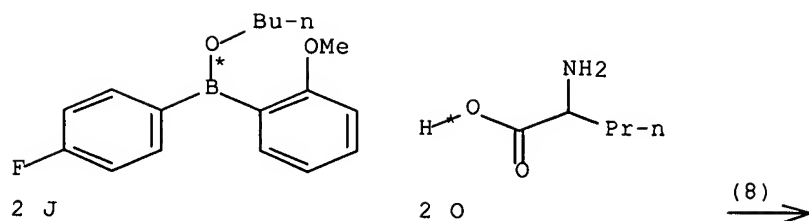


M
YIELD 71%



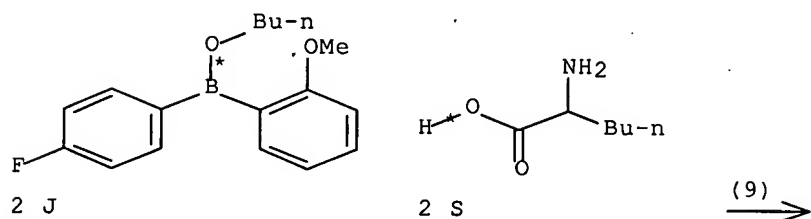
N
YIELD 71%

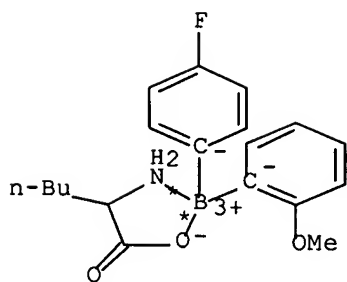
RX(8) OF 41 ...2 J + 2 O ==> Y + Z



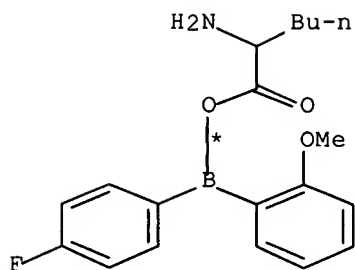
RX(8) RCT J 100689-51-8, O 760-78-1
 PRO Y 125869-40-1, Z 125553-34-6
 SOL 108-88-3 PhMe

RX(9) OF 41 ...2 J + 2 S ==> AA + AB





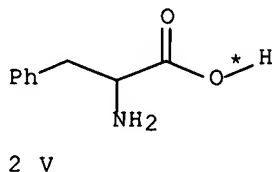
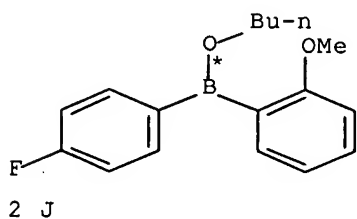
AA
YIELD 76%



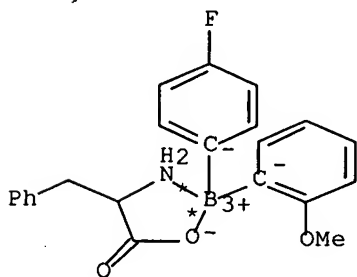
AB
YIELD 76%

RX(9) RCT J 100689-51-8, S 616-06-8
PRO AA 125842-44-6, AB 125553-35-7
SOL 108-88-3 PhMe

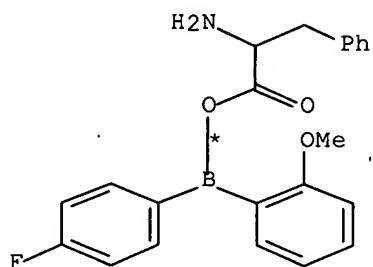
RX(10) OF 41 ...2 J + 2 V ==> AC + AD



(10) →



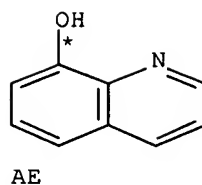
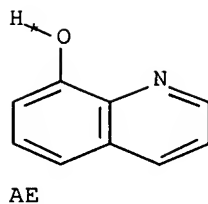
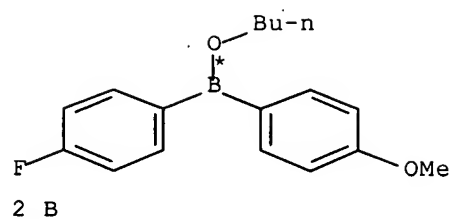
AC
YIELD 63%



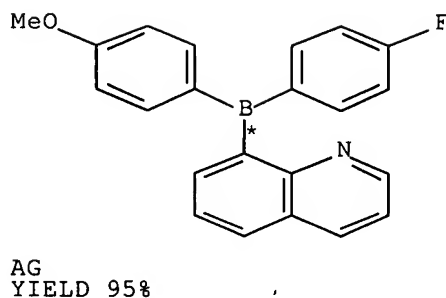
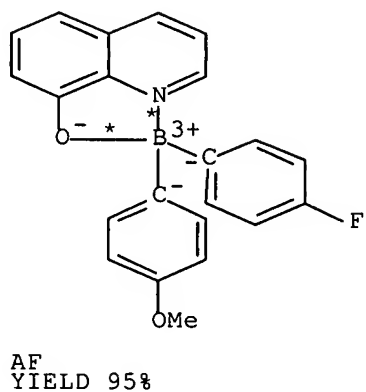
AD
YIELD 63%

RX(10) RCT J 100689-51-8, V 150-30-1
PRO AC 125842-45-7, AD 125553-36-8
SOL 108-88-3 PhMe

RX(11) OF 41 ...2 B + 2 AE ==> AF + AG

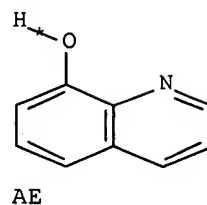
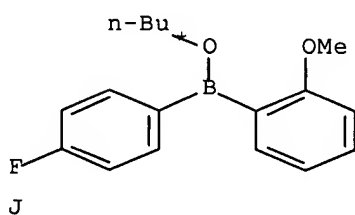
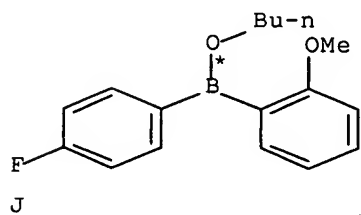


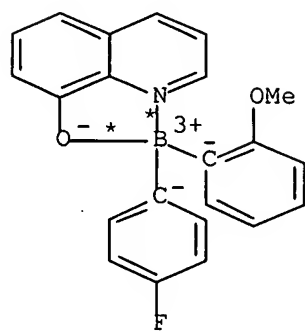
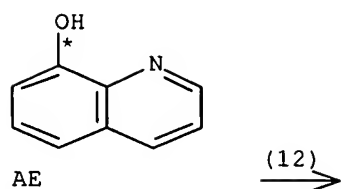
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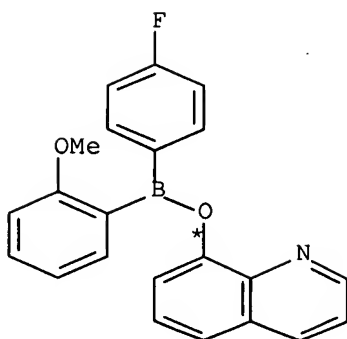
RX(11) RCT B 125553-26-6, AE 148-24-3
 PRO AF 125842-46-8, AG 125553-37-9
 SOL 64-17-5 EtOH

RX(12) OF 41 ... 2 J + 2 AE ==> AH + AI





AH
YIELD 94%



AI
YIELD 94%

RX(12) RCT J 100689-51-8, AE 148-24-3
 PRO AH 101754-10-3, AI 100689-52-9
 SOL 64-17-5 EtOH

L16 ANSWER 6 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:535001 CAPLUS Full-text

DOCUMENT NUMBER: 133:144898

TITLE: Organoboron compounds exhibiting anticoccidial activities

INVENTOR(S): Imazaki, Hideyuki; Fujikawa, Masazumi; Hayase, Yoshio; Kawaguchi, Harumoto

PATENT ASSIGNEE(S): Nitto Kasei Co., Ltd., Japan; Shionogi and Co., Ltd.

SOURCE: PCT Int. Appl., 100 pp.

CODEN: PIXXD2

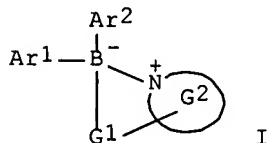
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000044387	A1	20000803	WO 1999-JP7139	19991220
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1155698	A1	20011121	EP 1999-959910	19991220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
PRIORITY APPLN. INFO.:			JP 1999-21822	A 19990129
			WO 1999-JP7139	W 19991220
OTHER SOURCE(S):		MARPAT 133:144898		
GI				



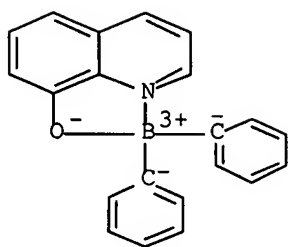
AB Drug compns. for animals (except Home sapiens), antiprotozoal agents and anticoccidial agents, containing compds. represented by general formula (I), salts of the same, or hydrates of both, wherein Ar1 and Ar2 are each independently an optionally substituted cyclic group; G1 is -A-, -A-CR1R2-, or -A-CR3R4-CR5R6-; and G2 is an optionally substituted azacyclic group (wherein the ring-constituting nitrogen atom is bonded to B-) or the like, provided the ring composed of B-, G1 and G2 is a five- or six-membered one.

IT 29190-60-1P 52997-17-8P 132722-17-9P
137001-21-9P 159097-99-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(organoboron compds. exhibiting anticoccidial and antiprotozoal activities)

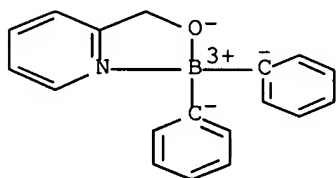
RN 29190-60-1 CAPLUS

CN Boron, diphenyl(8-quinolinolato-κN1,κO8)-, (T-4)- (9CI) (CA INDEX NAME)



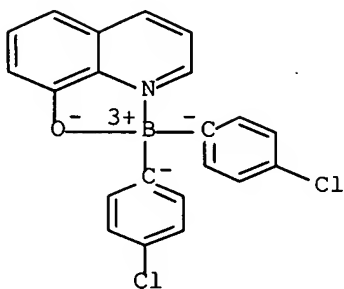
RN 52997-17-8 CAPLUS

CN Boron, diphenyl(2-pyridinemethanolato- κ N1, κ O2)-, (T-4)- (9CI)
(CA INDEX NAME)



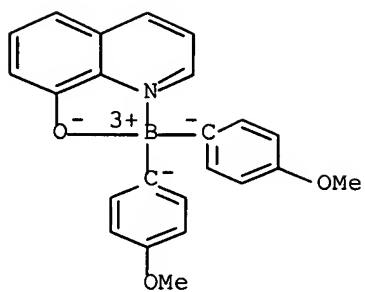
RN 132722-17-9 CAPLUS

CN Borón, bis(4-chlorophenyl)(8-quinolinolato- κ N1, κ O8)-, (T-4)-
(9CI) (CA INDEX NAME)



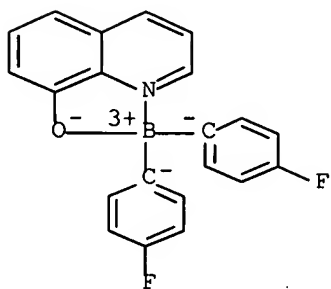
RN 137001-21-9 CAPLUS

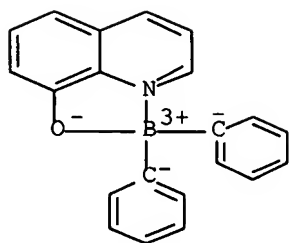
CN Boron, bis(4-methoxyphenyl)(8-quinolinolato- κ N1, κ O8)-, (T-4)-
(9CI) (CA INDEX NAME)



RN 159097-99-1 CAPLUS

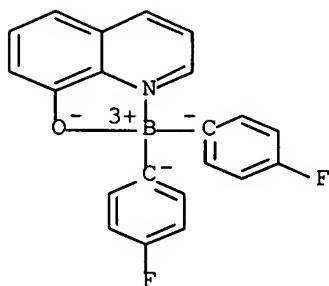
CN Boron, bis(4-fluorophenyl)(8-quinolinolato- κ N1, κ O8)-, (T-4)-
(9CI) (CA INDEX NAME)





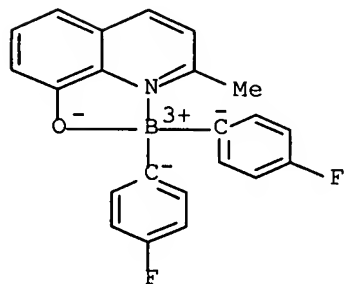
RN 159097-99-1 CAPLUS

CN Boron, bis(4-fluorophenyl)(8-quinolinolato-κN1,κO8)-, (T-4)-
(9CI) (CA INDEX NAME)



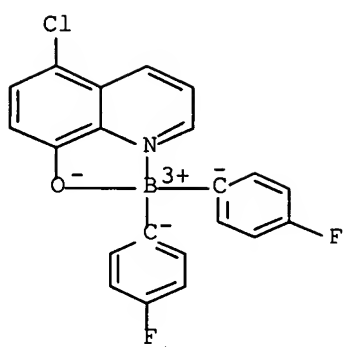
RN 159098-00-7 CAPLUS

CN Boron, bis(4-fluorophenyl)(2-methyl-8-quinolinolato-κN1,κO8)-,
(T-4)- (9CI) (CA INDEX NAME)



RN 159098-01-8 CAPLUS

CN Boron, (5-chloro-8-quinolinolato-κN1,κO8)bis(4-fluorophenyl)-,
(T-4)- (9CI) (CA INDEX NAME)



L16 ANSWER 13 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:332485 CAPLUS Full-text

DOCUMENT NUMBER: 120:332485

TITLE: Rotating-bomb combustion calorimetry and the standard enthalpies of formation of two borinic esters

AUTHOR(S): Torres, Luis Alfonso; Perez, Alejandro; Farfan, Norberto; Castillo, Dolores; Santillan, Rosa Luisa

CORPORATE SOURCE: Dep. Quim., Cent. Investigacion, Mexico City, 07000, Mex.

SOURCE: Journal of Chemical Thermodynamics (1994), 26(4), 337-43

CODEN: JCTDAF; ISSN: 0021-9614

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The standard massic energies of combustion of two borinic esters containing the intramol. $N \rightarrow B$ bond having different stabilities were determined by oxygen rotating-bomb combustion calorimetry. The studied compds. were: diphenyl(2-pyridylmethoxy-O,N)borane (A1) and di-Ph {2-(2'-pyridyl)ethoxy-O,N}borane (A2). Based on the exptl. results, the standard molar enthalpies of formation were determined as : $\Delta_f H_{mo}\{C_{18}H_{16}ONB(A1), cr\} = - (194.6 \pm 4.9) kJ \cdot mol^{-1}$ and $\Delta_f H_{mo}\{C_{19}H_{18}ONB(A2), cr\} = - (171.8 \pm 3.2) kJ \cdot mol^{-1}$.

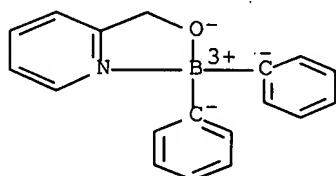
IT 52997-17-8

RL: PRP (Properties)

(heat of formation of, determination by rotating-bomb combustion calorimetry)

RN 52997-17-8 CAPLUS

CN Boron, diphenyl(2-pyridinemethanolato- $\kappa N1, \kappa O2$)-, (T-4)- (9CI)
(CA INDEX NAME)



ACCESSION NUMBER: 1991:619486 CAPLUS Full-text

DOCUMENT NUMBER: 115:219486

TITLE: Structure studies of bis(substituted)-2-(substituted)-8-hydroxyquinolines

AUTHOR(S): Liu, Xiaolan; Zhang, Xin; Miao, Fangming; Zhang, Shaohui; Lin, Kai; Zhang, Guomin; Han, Yuzhen; Xu, Xiaojie

CORPORATE SOURCE: Dep. Chem., Tianjin Normal Univ., Tianjin, 300074, Peop. Rep. China

SOURCE: Youji Huaxue (1991), 11(4), 410-15

CODEN: YCHHDX; ISSN: 0253-2786

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

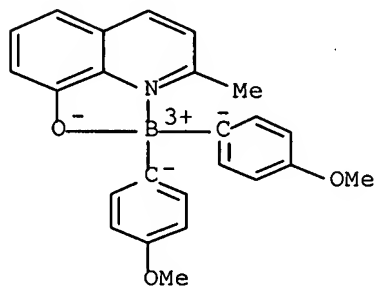
AB Bis(p-methoxyphenyl)-2-methyl-8-hydroxyquinoline borolactone (I) is orthorhombic, space group Pbca, with a 1.1741(5), b 1.6104(3), and c 2.1066(5) nm; Z = 8, R = 0.043. Bis(p-methoxyphenyl)-8-hydroxyquinoline borolactone (II) is monoclinic, space group P21/a, and a 1.0008(1), b 1.3956(2), c 1.3617(3)nm, and β 100.15(1) $^\circ$; Z = 4, R = 0.089. The structures of the 2 compds. were solved by direct method. The atoms of B, C(39), C(37), N and O(3) form a chelate ring with coordinated bond between B and N atoms. Dihedral angle between two benzenes is 57.8 $^\circ$ for I and 95.7 $^\circ$ for II. The bond order and charge d. from quantum chemical calcn. indicate the covalent nature of the bonds involving B atom. Atomic coordinates are given.

IT 137001-20-8 137001-21-9

RL: PRP (Properties)
(crystal structure of)

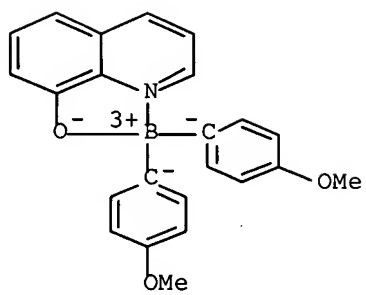
RN 137001-20-8 CAPLUS

CN Boron, bis(4-methoxyphenyl)(2-methyl-8-quinolinolato- κ N1, κ O8)-, (T-4)- (9CI) (CA INDEX NAME)

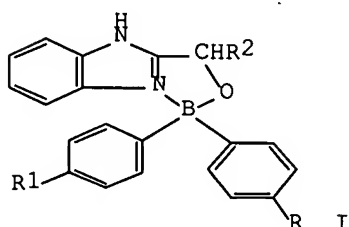


RN 137001-21-9 CAPLUS

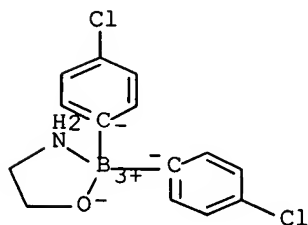
CN Boron, bis(4-methoxyphenyl)(8-quinolinolato- κ N1, κ O8)-, (T-4)- (9CI) (CA INDEX NAME)



L16 ANSWER 18 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1988:454817 CAPLUS Full-text
 DOCUMENT NUMBER: 109:54817
 TITLE: Boron compounds. (XIX). New organyloxydiarylborane
 chelates containing the virucide 2-(α -
 hydroxyalkyl)benzimidazole as ligands
 AUTHOR(S): Yuan, Guozheng; Li, Guiying; Zhang, Guomin
 CORPORATE SOURCE: Dep. Chem., Wuhan Univ., Guomin, Peop. Rep. China
 SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1987), 8(5), 398-402
 CODEN: KTHPDM; ISSN: 0251-0790
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 GI



AB Title compds. I (R, R1 = H, Me, Cl; R2 = H, Ph) were prepared through the
 reaction of 2-(α -hydroxymethyl)benzimidazole or 2-(α -hydroxybenzyl)-
 benzimidazole with diarylborinic acid. These compds. were identified by
 elemental anal., MS, IR and UV spectroscopies.
 IT 61731-73-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and hydrolysis of)
 RN 61731-73-5 CAPLUS
 CN Boron, [2-(amino- κ N)ethanolato- κ O]bis(4-chlorophenyl)-, (T-4)-
 (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1991:143497 CAPLUS Full-text

DOCUMENT NUMBER: 114:143497

TITLE: Proton and boron-11 NMR spectroscopy of diarylboron chelates containing boron-nitrogen coordinate bonds and of triboranes

AUTHOR(S): Yu, Dingzhang; Yuan, Guozheng; Zhang, Gumin

CORPORATE SOURCE: Dep. Anal. Test. Sci., Wuhan Univ., Wuhan, Peop. Rep. China

SOURCE: Fenxi Ceshi Tongbao (1990), 9(4), 5-10

CODEN: FCTOE8; ISSN: 1000-3800

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

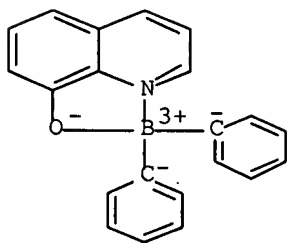
AB Spectroscopic characteristics of ^1H FT-NMR and FT-IR of 25 diarylboron chelates with 8-hydroxyquinoline, benzimidazole, ethanolamine or amino acids were reported. ^{11}B FT-NMR spectroscopy of $\text{Me}_4\text{N}^+ \text{B}_3\text{H}_8^-$ was described.

IT 29190-60-1 74344-31-3 132722-11-3
132722-17-9

RL: PRP (Properties)
(IR and NMR spectra of)

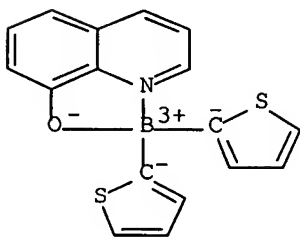
RN 29190-60-1 CAPLUS

CN Boron, diphenyl(8-quinolinolato- $\kappa\text{N}1, \kappa\text{O}8$)-, (T-4)- (9CI) (CA INDEX NAME)



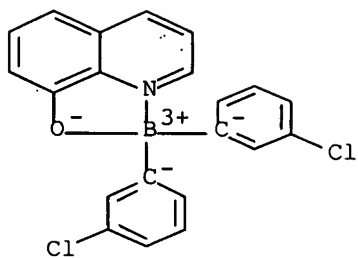
RN 74344-31-3 CAPLUS

CN Boron, (8-quinolinolato- $\kappa\text{N}1, \kappa\text{O}8$)di-2-thienyl-, (T-4)- (9CI)
(CA INDEX NAME)



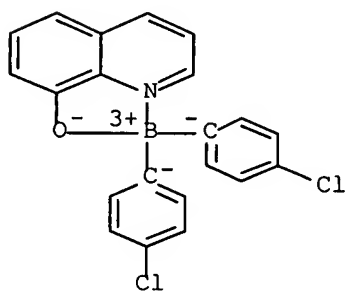
RN 132722-11-3 CAPLUS

CN Boron, bis(3-chlorophenyl)(8-quinolinolato- $\kappa\text{N}1, \kappa\text{O}8$)-, (T-4)-
(9CI) (CA INDEX NAME)



RN 132722-17-9 CAPLUS

CN Boron, bis(4-chlorophenyl) (8-quinolinolato-κN1,κO8)-, (T-4)-(9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1974:528040 CAPLUS Full-text

DOCUMENT NUMBER: 81:128040

TITLE: Crystal and molecular structure of
B,B-bis(p-fluorophenyl)boroxazolidine,
(p-FC₆H₄)₂BO(CH₂)₂NH₂

AUTHOR(S): Rettig, Steven J.; Trotter, James

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC,
Can.

SOURCE: Acta Crystallographica, Section B: Structural
Crystallography and Crystal Chemistry (1974), B30, Pt.
9, 2139-45

CODEN: ACBCAR; ISSN: 0567-7408

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. Crystals of the title compound are orthorhombic with lattice parameters a 13.442(4), b 10.214(3), c 9.283(2) Å, Z = 4, space group P2₁2₁2₁. The structure was solved by direct methods, and refined by electron-d. and full-matrix least-squares procedures to R = 0.047 for 1234 reflections. The 5-membered borox-azolidine ring is in a distorted half-chair conformation. Bond angles in the ring range from 99.9(2)° for OBN to 108.2(2)° for BOC. Bond lengths are: mean B-C 1.618(3), B-N 1.652(4), B-O 1.471(4), C-N 1.491(4), C-O 1.418(4), mean C-F 1.371(4), mean C-C(aromatic) 1.390(13), and C(sp³)-C(sp³) 1.494(6) Å. The structure consists of discrete mols. each linked to 6 others by an extensive network of O...H-N(O...N = 2.941(3) Å, F...H-N-(F...N = 3.171(4) Å, and F...H-C(F...C = 3.318(5) Å) hydrogen bonds.

IT **25610-36-0**

RL: PRP (Properties)
(crystal structure of)

RN 25610-36-0 CAPLUS

CN Boron, [2-(amino-κN)ethanolato-κO]bis(4-fluorophenyl)-, (T-4)-
(9CI) (CA INDEX NAME)

